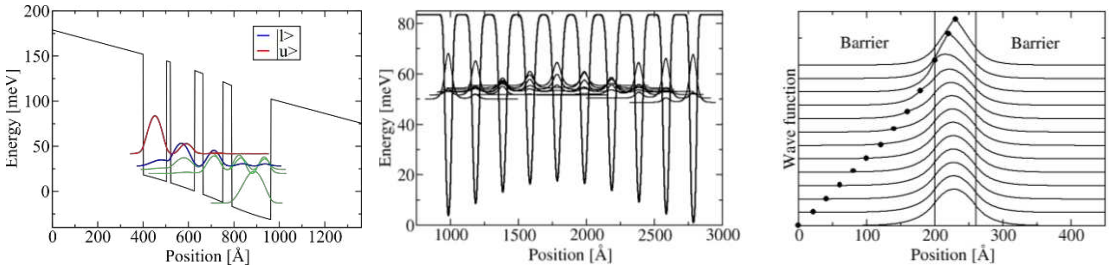
# Open-source bandstructure models of interdiffusion, impurity and exciton states for the Quantum Wells, Wires and Dots (QWWAD) simulation suite

**Alexander Valavanis[1,*] Andrew Grier[1], Jonathan D. Cooper[1], Craig A. Evans[1], and Paul Harrison[2]**

[1] School of Electronic and Electrical Engineering, University of Leeds, Leeds LS2 9JT, U.K.
[2] Materials and Engineering Research Institute, Sheffield Hallam University, Sheffield S1 1WB, U.K.
*Contact Email: a.valavanis@leeds.ac.uk

The vast majority of high-quality software for simulating semiconductor nanostructures (e.g., [1]) is supplied under a proprietary license and its source code cannot be studied, modified or redistributed by its users. The open-source project, Quantum Wells, Wires and Dots (QWWAD) [2] is a free, non-commercial community-focused resource, which accompanies the new 4th edition of the eponymous textbook [3]. Previously described features in QWWAD include numerical Schrodinger/Poisson solvers in generic 1D potentials [e.g., Fig. 1(a)], quasi-analytical and empirical pseudopotential calculations of the band-structure in quantum wires and dots, and scattering calculations for interactions with impurities, phonons, interface roughness, alloy disorder and carrier–carrier processes. We describe new tools, included in the latest release (QWWAD v1.4), for modelling the perturbed quantum-confined states within 2D heterostructures resulting from interdiffusion, impurities and excitonic contributions.




(a) (b) (c)

**Fig. 1**: (a) Self-consistent Poisson–Schrödinger solution for a THz QCL using tight-binding boundary conditions. (b) Potential profile (bold) and electron probability densities (feint) in a multi-quantum-well system after simulated annealing, using a constant diffusion coefficient. (c) Wave functions for 1s state of an electron interacting with a donor at a range of locations (indicated by circles) within a quantum well, assuming a spherically symmetrical hydrogenic factor.

In QWWAD v1.4, diffuse bandstructure is simulated using numerical solutions to a Fick annealing model, with the diffusion coefficient being either constant or a function of diffusant concentration, time or position within the heterostructure [Fig. 1(b)]. Quasi-analytical models of 1s-states for impurities in heterostructures (with cylindrically, spherically or ellipsoidally symmetric orbitals) [Fig. 1(c)]. Numerical variational solvers enable the calculation of higher-order s- and p-states. Excitonic states are also computed using a similar set of models.

Development of QWWAD is coordinated through a community-focused project on the Launchpad website [3]. A hierarchical software architecture allows considerable flexibility in its usage, including a C++ Application Programmers Interface, "building-block" programs for common modelling tasks and a set of example UNIX scripts suitable for non-expert users.

[1] Nextnano, http://www.nextnano.de
[2] Quantum wells, wires and dots (QWWAD), http://launchpad.net/qwwad
[3] P. Harrison and A. Valavanis, Quantum Wells, Wires and Dots, 4th Ed. Wiley, Chichester (2016).